

Scientific Report

on the

Exchange Grant

“Influence of material solubility effects on photovoltaic performance of low band-gap conjugated polymers blended with various fullerene derivatives”

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1. Purpose of the visit

Organic solar cells show steadily increasing power conversion efficiencies approaching 5-6% according to the recent reports. All advanced material combinations that yield power conversion efficiencies above 4.5-5.0% are based on low band-gap conjugated polymers. Design of well-performing low band-gap polymers is a great challenge for material chemists working in the area of organic photovoltaics. Among several hundreds of investigated low band gap polymers just few remarkable examples showed superior photovoltaic performances in comparison with conventional material combinations (e. g. P3HT/PCBM). It is not clear why some polymers work well in organic solar cells while many others do not give any reasonable photovoltaic characteristics.

We have shown recently that all parameters of the poly(3-hexylthiophene)-based bulk heterojunction organic solar cells depend strongly on the solubility of the fullerene derivative used as electron acceptor component. It is very likely that similar solubility-related effects take place in the case of novel material combinations comprising low band gap polymers. Therefore it becomes mandatory to investigate material structure-solubility-photovoltaic performance relationships for low band-gap polymer systems. In the frame of the present project we planed to investigate few low band-gap polymers (Figure 1). Some of these polymers were synthesized in our group at IPCP RAS (Chernogolovka), some others were provided by collaborators from ISPM RAS (Moscow).

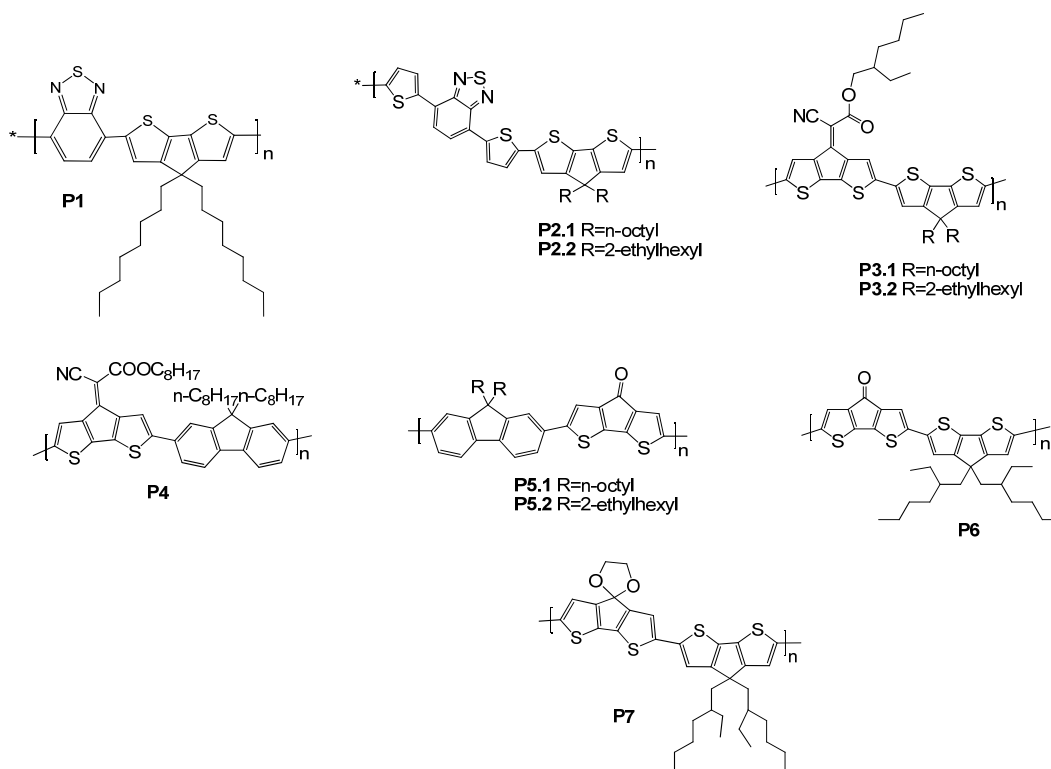


Figure 1 Molecular structures of the investigated low band gap donor polymers

2. Description of the work carried out during the visit

Initially all studied polymers were combined with conventional fullerene-based material [60]PCBM. Obtained PCBM/polymer composites with variable component ratios were investigated as active layer materials in organic solar cells (layout of the cell is shown in Figure 2). This preliminary test allowed us to get some impression about photovoltaic performance of all materials. On the next step the most promising polymer was combined with various fullerene derivatives possessing different solubilities in organic solvents. Variation of the fullerene-based material allowed us to manipulate active layer morphology.

All studies performed in the frame of the visit to LIOS can be summarized as follows.

- Comparative study of all low band-gap polymers in solar cells together with [60]PCBM as electron acceptor material.
- Investigation of the best-performing low band-gap polymer in combination with series of fullerene derivatives possessing different solubilities.
- Evaluation of the active layer morphology for all investigated composites using optical and AFM microscopy.

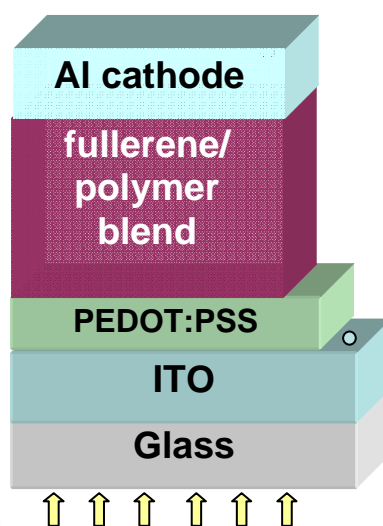


Figure 2 Layout of the investigated bulk heterojunction organic solar cell

3. Description of the main results obtained

3.1 Comparative study of all low band-gap polymers in solar cells together with [60]PCBM as electron acceptor material

Output parameters of organic solar cells comprising polymers **P1-P7** are summarized in Table 1. It is seen from these data that only one polymer **P2.1** showed power conversion efficiencies above 2.0% in combination with [60]PCBM. All other polymers showed much lower performances that might be a consequence of their unfavorable molecular structures and compositions or their insufficient purity. Some low molecular weight impurities might seriously affect thermal stability of the blends and their nanomorphology. Catalyst impurities or traces of some reactive organic reagents might work as efficient charge traps thus inhibiting photocurrent generation. Device fill factors might also fall down in this case because of the accumulation of the trapped charges in the active layer.

Investigation of possible factors responsible for low photovoltaic performance of the polymers will be done in the future in close cooperation with synthetic chemists who provided us these materials. We focused our further studies on the polymer **P2.1** since it can be considered as the most promising electron donor material among the structures shown in Figure 1.

Table 1. Output parameters of organic solar cells comprising polymers **P1-P7**

Polymer	Optimal P:PCBM weight ratio	I _{sc} , mA/cm ²	V _{oc} , mV	FF, %	η, %
P1	1:3	5.0	600	33	1.0
P2.1	1:2	10.1	500	45	2.4
P2.2	1:2	4.5	500	32	0.7
P3.1	1:2	0.13	350	42	0.02
P3.2	1:2	0.01	300	17	0.0005
P4	1:4	0.23	800	36	0.07
P5.1	1:3	0.19	650	29	0.035
P5.2	1:4	0.36	800	30	0.08
P6	1:2	0.95	600	27	0.15
P7	1:3	2.94	560	32	0.53

3.2 Investigation of the best-performing low band-gap polymer P2.1 in combination with series of fullerene derivatives possessing different solubilities

In this part of work we applied a family of 12 fullerene derivatives possessing different solubilities as electron acceptor counterparts for blending with the polymer **P2.1**. Molecular structures of these compounds are not shown in this report (publication is planned).

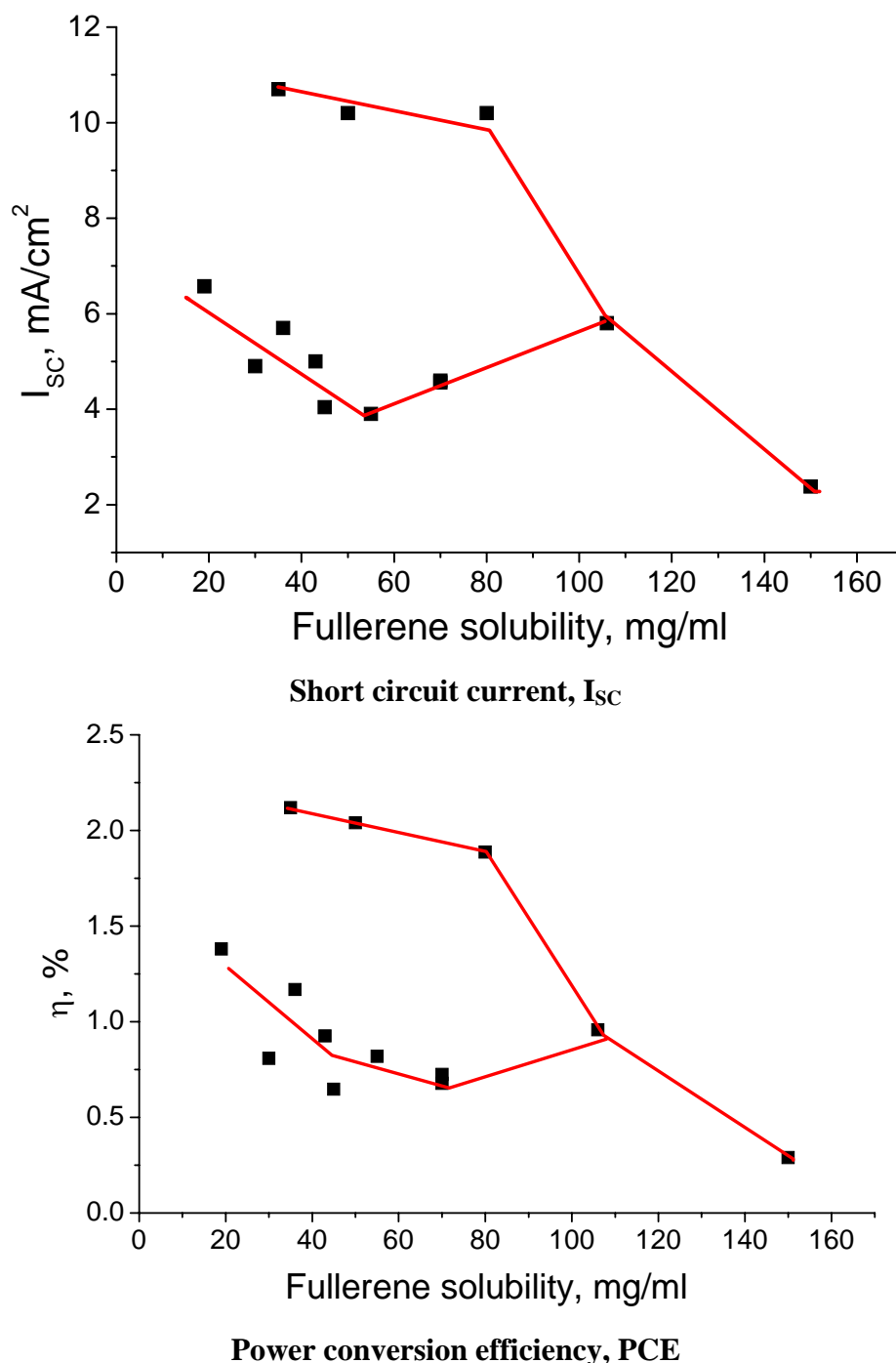


Figure 3 Output parameters of solar cells comprising polymer **P2.1** and various fullerene derivatives as a function of the solubility of the fullerene component

We expected to observe some solubility dependence with a single maximum similar to the one previously revealed for P3HT-based composites [1]. However, experimental study provided different results. To our great surprise, polymer **P2.1** exhibited very unusual double-branch type solubility dependence shown in Figure 3. These results were reproduced several times that confirms that the observed double branch behavior cannot be an experimental error.

The obtained results suggest that some fullerene derivatives are better compatible with the polymer than others. This compatibility seems to be independent on the solubility of the fullerene-based material and, most probably, is dictated by some peculiarities of their molecular structures.

3.3 Evaluation of the active layer morphology for all investigated composites using optical and AFM microscopy

In order to understand the observed double-branch type solubility behavior we performed AFM studies for all prepared fullerene/polymer composites. However, AFM studies revealed no substantial differences in the surface topology of the investigated blends (Figure 4). In spite of the very similar surface topologies, it is very likely that these blends have different bulk morphologies that can be investigated using some other microscopy techniques (perhaps, TEM) penetrating deeper into (or even through) organic films. We will look for opportunity to apply such techniques for investigation of our systems in future.

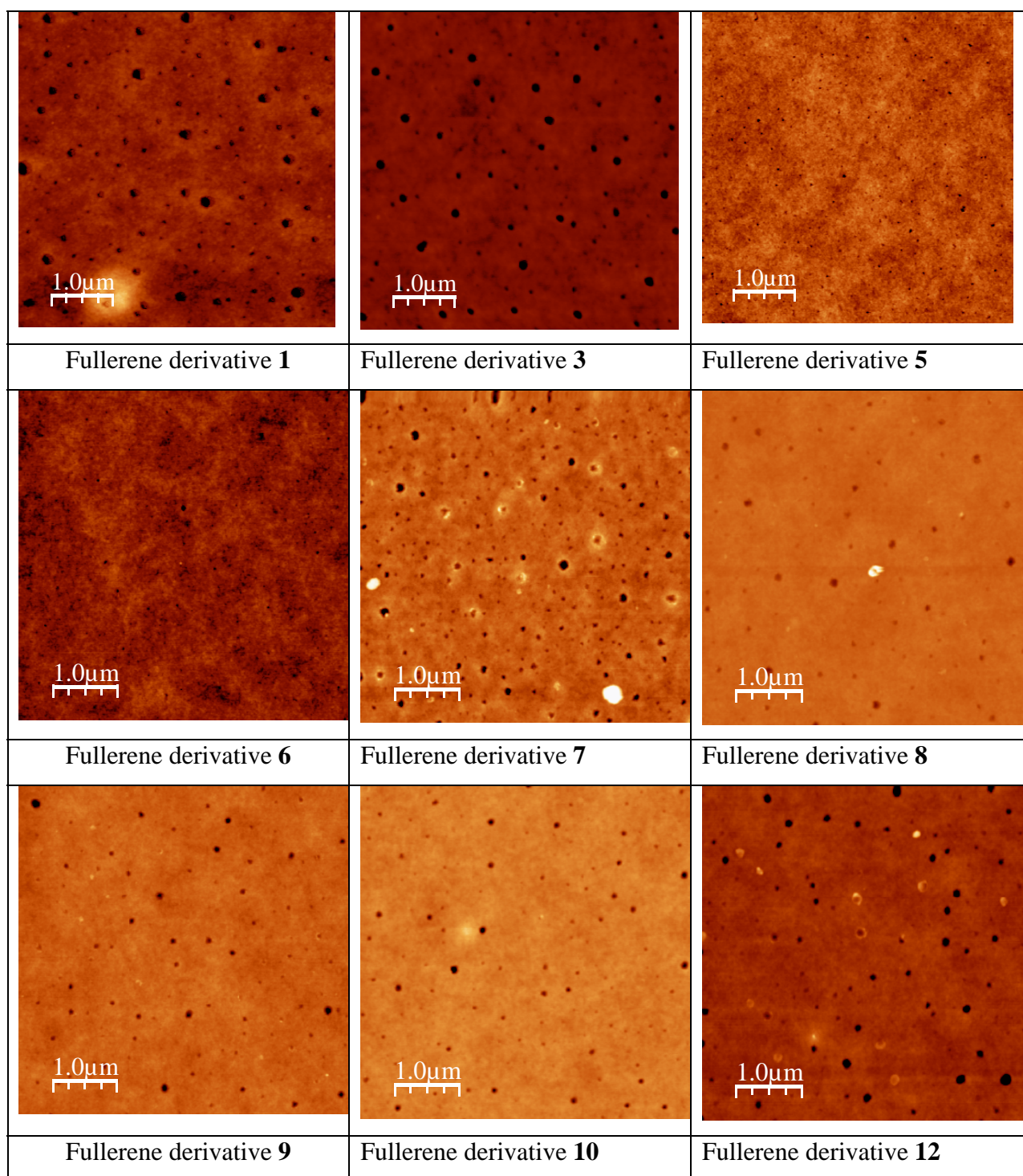


Figure 4 AFM topology images of the blends composed of the polymer **P2.1** and different fullerene derivatives

References

1. P. A. Troshin, H. Hoppe, J. Renz, M. Egginger, J. Yu. Mayorova, A. E. Goryachev, A. S. Peregudov, R.N. Lyubovskaya, G. Gobsch, N. S. Sariciftci, V. F. Razumov. Material solubility-photovoltaic performance relationship in design of novel fullerene derivatives for bulk heterojunction solar cells. *Adv. Funct. Mater.* **2009**, 19, 779–788

Future collaboration with host institution

We obtained quite promising results regarding to the solubility behavior of the blends composed of the polymer **P2.1** and various fullerene derivatives. It was revealed that fullerene derivative molecular structure is one of the most important parameters that should be optimized to achieve desired compatibility and miscibility of the components in the photoactive blends. At the same time, good compatibility of the donor and acceptor materials results in enhanced photovoltaic performance of the blends. Therefore, engineering of the fullerene derivative structure might be considered as one of the most efficient ways to improve performance of organic solar cells based on novel low band-gap polymers.

Our further collaboration with LIOS will be focused on the following issues.

1. Investigation of the factors responsible for poor photovoltaic performance of the developed low band gap polymers (problems of unfavorable molecular structure or insufficient purity).
2. Investigation of the solubility trend for other low band gap polymers that are currently being synthesized at IPCP RAS and LIOS.
3. Systematic study will be directed on elaboration of a structure-property relationship model that should allow one to predict compatibility of any couple of donor and acceptor materials just considering their molecular structures.

Projected publications

Results of this work will be presented as a part of a larger manuscript that might be submitted to *Advanced Functional Materials*. Preliminary results will be also included to the presentations at the conferences TPE 2010 in Rudolstadt and EMRS Spring Meeting 2010 in Strasbourg.

Acknowledgements

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